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Subject: Release Notification: MILAGRO–1_2_0

Executive Summary

We wish to announce the release 1_2_0 of MILAGRO, the three-dimensional, XYZ Implicit Monte Carlo code for radiative transfer. This release of MILAGRO has a constant material volume source capability. This capability was not fully implemented in previous versions and never tested. We derive a simple equilibrium diffusion solution in an infinite medium as an analytical benchmark to which we can compare MILAGRO results. Indeed, our new MILAGRO results agree fairly well with the benchmark. Finally, we have added a few simple relevant problems to the nightly regression test suite.

1. Introduction

In the Fleck and Cummings algorithm [1], a time-explicit portion of an external material volume source stays with the material equation, and the remaining "time-implicit" portion goes directly to the radiation equation. The external material volume source in Milagro-1_0_0 [2, 3] and Milagro-1_1_0 [4] was only partially implemented; we had only included the "time-implicit" portion. We have corrected that oversight with this release, Milagro-1_2_0.

2. Radiation and Material Equations

Here, we merely reproduce the gray radiation and material equations from Fleck and Cummings [1]. The equations we wish to solve are

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I = \sigma\Big(\frac{c}{4\pi}\phi - I\Big) \,, \tag{1}$$

$$\frac{\partial \mathcal{E}}{\partial t} = \sigma\Big(\int I \, d\Omega - c\phi\Big) + Q \;\;, \tag{2}$$

where I is the specific intensity, $\mathcal{E}$ is the material energy, $\phi = aT^4$ is the equilibrium energy density, and Q[energy/time/volume] is the external material volume source in question. The derivation of the Fleck and Cummings method yields the Implicit Monte Carlo (IMC) equations:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I + \sigma I = \frac{c}{4\pi} f \sigma \phi^n + \frac{1}{4\pi}(1-f)\sigma \int I \, d\Omega + \frac{1}{4\pi}(1-f)Q \ \ , \tag{3}$$

$$\frac{\partial \mathcal{E}}{\partial t} = f\sigma \int I \, d\Omega - c f \sigma \phi^n + fQ \ \ , \tag{4}$$

where ϕ^n is the equilibrium radiation energy density at the beginning of the timestep and f is the so-called Fleck factor which ranges from one for a fully time-explicit calculation to approaching zero for a "fully" time-implicit calculation. (We say "fully" to indicate that the Fleck and Cummings IMC method is not fully implicit [5].)

3. Equilibrium Diffusion in an Infinite Medium

We desire a simple benchmark problem to which we can compare Milagro results. Let us consider equilibrium diffusion [6] in an infinite, homogeneous medium (i.e., no spatial derivatives),

$$(C_v + 4aT^3)\frac{\partial T}{\partial t} = Q \ \ , \tag{5}$$

where C_v is the heat capacity in units of [energy/volume/temperature], a=0.01372 jks/cm^3/keV^4 is the radiation constant, T is the equilibrium temperature, t is time, and Q is, again, a constant external material volume source in [energy/volume/time].

In order to solve Eq. 5, we recognize that, using the chain rule, the left hand side can also be written as

$$(C_v + 4aT^3)\frac{\partial T}{\partial t} = \frac{\partial}{\partial t}(aT^4 + C_v T + k) \ \ , \tag{6}$$

where k is a constant of integration to be determined. Substituting Eq. 6 into Eq. 5, we have

$$\frac{\partial}{\partial t}(aT^4 + C_v T + k) = Q \ \ . \tag{7}$$

Integrating from $t = 0$ to $t = \tau$, we obtain

$$aT^4 + C_v T + k = Q\tau \ \ , \tag{8}$$

where we have absorbed another constant of integration into k. We determine k by evaluating Eq. 8 at time $\tau = 0$ and, calling T_0 the temperature at time $\tau = 0$, we find that

$$k = -(aT_0^4 + C_v T_0) \ \ . \tag{9}$$

Substituting k into Eq. 8 and rearranging, we arrive at an equation for the temperature T for a given time τ,

$$T^4 + \frac{C_v}{a}T + (-T_0^4 - \frac{C_v}{a}T_0 - \frac{Q}{a}\tau) = 0 \ \ . \tag{10}$$

4. Infinite Medium, Equilibrium Diffusion Benchmark

Let us consider an infinite medium system where, initially, both the temperatures and energies are equivalent for both radiation and material. From $C_v T_0 = aT_0^4$, we find that $T_0 = 0.89994$ keV for $C_v = 0.01$ jks/cm^3/keV. Let us consider the temperature at 0.1 shakes for a source of 10.0 jks/cm^3/sh. Using the root-finder in Mark Gray's Analytical Test Suite[1], we determine $T_{0.1} =$ 2.9137 keV.

5. Milagro Specifications and Results

In Milagro, we mocked up the infinite medium with one cell and all boundaries reflecting. We used unit density, an absorption coefficient of 100 cm^2/g, 1000 particles, and a timestep of 0.001 sh. We ran Milagro twenty times, each with a different random number seed. Figure 1 shows the average radiation and material temperatures along with their respective one-standard-deviation error bars plotted against the analytic solution. At 0.1 sh, the radiation temperature was 2.9099 keV ($\sigma = 0.0049$) and the material temperature was 2.9102 keV ($\sigma = 0.0049$). Both the radiation and material temperatures are within one standard deviation (0.78 and 0.71, respectively) of the analytical temperature.

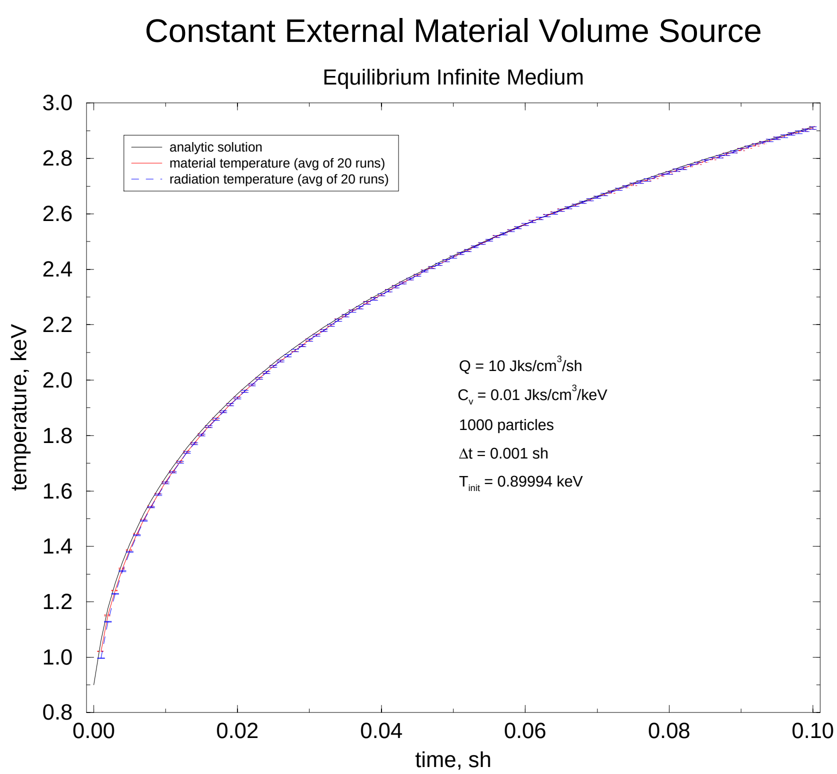

FIG. 1: The equilibrium temperature for a constant external material volume source.

[1] The Analytical Test Suite is an X–6 application used to verify radiation transport packages.

We were a little concerned that the material temperature was always higher than the radiation temperature. It turns out that this behavior is an issue independent of the external material volume source and is, in fact, due to the energy-weight cutoff. When a particle's energy-weight decreases to 0.01 times its original energy-weight, it is killed, and all of its energy is deposited to the material. This feature, which we affectionately call "Full-Clip Russian Roulette," is intended to reduce computational time at the expense of a small bias in the distribution of energy.

In order to study the effects of the energy-weight cutoff independently of the source, we run a problem similar to the specified benchmark, but without the external material volume source. This problem is a coupled, steady-state problem. For ten independent runs, the results show the radiation temperature at 0.9157 keV ($\sigma = 0.0094$) and the material temperature at 0.9184 keV ($\sigma = 0.0095$). Now, if we decrease the energy-weight cutoff fraction to 0.001 and run ten more independent runs, we obtain an average radiation temperature of 0.9044 keV ($\sigma = 0.0086$) and an average material temperature of 0.9047 keV ($\sigma = 0.0086$). Indeed, dropping the minimun energy-weight cutoff fraction diminished the difference between the material and radiation temperatures. We demonstrate these differences between the material and radiation temperature in Figure 2. Incidentally, dropping the minimum energy-weight cutoff fraction did not increase the run-time probably because the large opacity and small Fleck factor cause particles to be short-lived. Additionally, the census particle comb tends to reduce small-weighted particles at the beginning of each timestep.

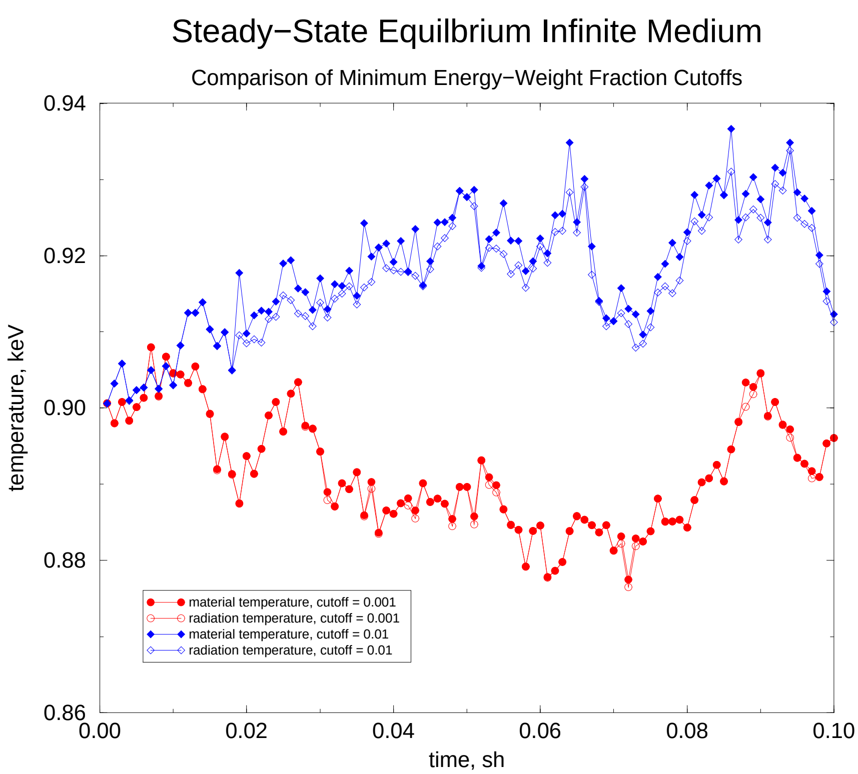

FIG. 2: Non-equilibrium temperatures from too large of an energy-weight fraction cutoff.

TABLE 1: Draco packages used in Milagro-1_2_0.

Package	Release
`ds++`	1_0_0
`c4`	1_0_0
`rng`	1_1_0
`mc`	1_1_0
`imc`	1_2_1

6. Verification and Regression Tests

We have devised two simple verification/regression problems to test the external material volume source. These tests are simple and fast so they can be run in the nightly regression tests. The first one considers a totally decoupled system, which is carried out with an opacity of zero. All the energy goes into the material. The second one is a version of the analytic problem, toned-down with fewer particles and time steps. The results for both have been verified by hand and incorporated into the regression test suite.

7. Package Dependencies

Milagro-1_2_0 uses the same Draco components as Milagro-1_0_0 [3] and Milagro-1_1_0 [4]. However, the new version of Milagro utilizes updated or branched releases of some of those packages. Table 1 lists the packages that are used in Milagro-1_2_0. Note that all of these packages are currently in a `last_stable` state, except for the imc package, which is a branch. Currently, the `last_stable` release of the imc package is imc-1_2_0, but it contains an error in the external material volume source that was corrected in the branch. Release imc-2_0_0, due shortly, will contain the corrections.

The current code modifications were made only to Source_Init and Global_Tally. Modifications to Parallel_Source_Init will be deferred until major release 2, which is expected soon.

8. Conclusion

We have implemented a constant, external material volume source into Milagro and released it as Milagro-1_2_0. Previously, only the "time-implicit" portion of the source was implemented, and it was never tested (it would have failed).

We have derived a simple, infinite-medium, equilibrium diffusion solution with a constant, external material volume source. Our results compared favorably to this analytic result. One discrepancy was that the material and radiation temperatures appeared to come out of equilibrium and become offset from each other. We discovered that this discrepancy was due to the minimum energy-weight fraction cutoff. With the discrepancy explained, we consider the constant external material volume source to be verified in Milagro-1_2_0. Future work may involve improving this "Full-Clip Russian Roulette."

We have added two more simple test problems to the regression test suite.

References

[1] J. A. Fleck, Jr. and J. D. Cummings, "An implicit Monte Carlo scheme for calculating time and frequency dependent nonlinear radiation transport," *Journal of Computational Physics*, vol. 8, pp. 313–342, 1971.

[2] T. M. Evans and T. J. Urbatsch, "MILAGRO: A parallel Implicit Monte Carlo code for 3-d radiative transfer (U)," in *Proceedings of the Nuclear Explosives Code Development Conference*, (Las Vegas, NV), Oct. 1998. LA-UR-98–4722.

[3] T. Urbatsch and T. M. Evans, "Release notification: MILAGRO-1_0_0," Research Note XTM:RN(U)99-016, Los Alamos National Laboratory, June 4, 1999. LA-UR-2948.

[4] T. Urbatsch and T. Evans, "Release notification: MILAGRO-1_1_0," Research Note X–6:RN(U)-99-033, Los Alamos National Laboratory, October 26 1999. LA-UR-99-5694.

[5] E. W. Larsen and B. Mercier, "Analysis of a Monte Carlo method for nonlinear radiative transfer," *Journal of Computational Physics*, vol. 71, pp. 50–64, 1987.

[6] J. E. Morel, T. A. Wareing, and K. Smith, "A linear-discontinuous spatial differencing scheme for S_N radiative transfer calculations," *Journal of Computational Physics*, vol. 128, pp. 445–462, 1996.

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